

Molecular conformation and electronic structure From molecular switches to chiral heterorecognition

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In order to understand molecular function we have to know how the molecular shape and its orientation are changing. On surfaces the conformation is determined by preferential adsorption sites, which impose orientation, changes in chemical state and shape of the molecule and the surface. The chemical state is seen by X-ray photoelectron spectroscopy (XPS), while the corresponding angular resolved diffraction experiment (XPD) maps the angles of molecular bonds with high accuracy. The examples of chiral heterorecognition of D- and L-cysteine on a chiral gold surface and the reorientation of C60 molecules upon charge transfer are presented. For the model system of one monolayer of C60 on h-BN/Ni(111) a peculiarly strong charge transfer is found upon onset of molecular rocking motion. This is observed by strong changes in temperature dependent valence band photoemission (UPS) [1].

[1] Muntwiler et al. Phys. Rev. B 71 (2005) 241401.